WHERE AND WHY THE GENERALIZED HAMILTON-JACOBI REPRESENTATION DESCRIBES MICROSTATES OF THE SCHRÖDINGER WAVE FUNCTION

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A generalized Hamilton-Jacobi representation describes microstates of the Schrödinger wave function for bound states. At the very points that boundary values are applied to the bound state Schrödinger wave function, the generalized Hamilton-Jacobi equation for quantum mechanics exhibits a nodal singularity. For initial value problems, the two representations are equivalent.

1. INTRODUCTION

The Schrödinger equation is a linear differential equation. Consequently, the Schrödinger representation of quantum mechanics is well development and most familiar. In the early days of quantum mechanics, the physics community had considered that in one dimension an equivalent representation of quantum mechanics was rendered by a generalized Hamilton-Jacobi equation [1–3] or the related Milne [4] or Pinney [5] equation. These equations are nonlinear differential equations. Consequently, their development as a representation of quantum mechanics is not as extensive. Yet, some workers have noted various computational advantages for directly solving the generalized Hamilton-Jacobi representation or its equivalent rather than solving the Schrödinger representation [4,6–10]. Even today familiarity with the generalized Hamilton- Jacobi representation ends for most other workers with the WKB approximation where the higher order terms of the generalized Hamilton-Jacobi equation have been ignored. There still is a widely held perception that the generalized Hamilton-Jacobi representation is at best only equivalent to the Schrödinger representation and offers nothing new.

With regard to the foundations of quantum mechanics, recent progress in the generalized Hamilton-Jacobi representation has shown that this representation sometimes, albeit not always, renders microstates of the Schrödinger wave function. On the one hand, the generalized Hamilton-Jacobi representation of bound states has shown that each of various, non-unique trajectories in phase space for energy E is consistent with the unique eigenfunction of energy E of the Schrödinger representation [11]. Each of these distinct trajectories determines a microstate of the Schrödinger wave function [11]. These trajectories differ with possible Feynman paths. Each trajectory or microstate alone determines the Schrödinger wave function in contrast to Feynman's giving equal weight to all possible paths whose phases are subject to a classical generator of the motion. These microstates undermine the widely held belief that the Schrödinger wave function be an exhaustive description of quantum phenomena. On the other hand, the phase-space trajectory for tunneling or reflection and transmission problems does not manifest any microstates for the trajectory is unique and consistent with the unique Schrödinger wave function [12,13].

Herein, we resolve why a generalized Hamilton-Jacobi representation only sometimes describes microstates for the Schrödinger wave function of nonrelativistic quantum mechanics. The reasons are mathematical. We investigate the Schrödinger and generalized Hamilton-Jacobi representations in one dimension and make limited extensions to higher dimensions. We consider the time-independent case for both initial condition and boundary value problems. As a byproduct, the Schrödinger equation and the generalized Hamilton-Jacobi equations are shown not to be equivalent of each other. In this investigation, we examine the consequences of using a generalized Hamilton-Jacobi equation rather than the Milne or Pinney equation to describe quantum phenomena. This choice was arbitrary as we would have produced the same findings by using the Milne or Pinney equation.

2. THEORY

Before we examine specific cases, we present established relationships between the solutions for generalized Hamilton-Jacobi equation and the Schrödinger equation. The generalized Hamilton-Jacobi equation for quantum mechanics is given in one dimension x by [3]

$$\frac{(W')^2}{2m} + V - E = -\frac{\hbar^2}{4m}\left[\frac{W'''}{W'} - \frac{3}{2}\left(\frac{W''}{W'}\right)^2\right],\tag{1}$$

where W is Hamilton's characteristic function, W' is the momentum conjugate to x, V is the potential, E is energy, m is the mass of the particle, and $\hbar = h/(2\pi)$ where in turn h is Planck's constant. The left side of Eq. (1) manifests the classical Hamilton-Jacobi equation which renders the generator of motion for Feynman paths. The right side of Eq. (1) is the Schwarzian derivative which manifests the quantum effects.

We explicitly note that W and W' are real even in the classically forbidden region. The general solution for W' is given by [11]

$$W' = \pm(2m)^{1/2}(a\phi^2 + b\theta^2 + c\phi\theta)^{-1},\tag{2}$$

where (a,b,c) is a set of real coefficients such that $a, b > 0$, and (ϕ, θ) is a set of normalized independent solutions of the associated time-independent Schrödinger equation, $-\hbar^2\psi''/(2m) + (V - E)\psi = 0$. The independent solutions (ϕ, θ) are normalized so that their Wronskian, $\mathcal{W}(\phi, \theta) = \phi\theta' - \phi'\theta$, is scaled to give $\mathcal{W}^2(\phi, \theta) = 2m/[\hbar^2(ab - c^2/4)] > 0$. This ensures that $(a\phi^2 + b\theta^2 + c\phi\theta) > 0$. We note for completeness that a particular set (ϕ, θ) of independent solutions of the Schrödinger equation may be chosen by the superposition principle such that the coefficient c is zero. The $\pm$ sign in Eq. (2) designates that the motion may be in either x-direction. Hereon, we shall assume motion in the $+x$-direction. The corresponding solution for the generalized Hamilton's characteristic function, W, which is also a generator of the motion, is given by

$$W = \hbar \arctan\left(\frac{b(\theta/\phi) + c/2}{(ab - c^2/4)^{1/2}}\right) + K,$$

where K is an integration constant which we may set to zero herein.

We now show that (ϕ, θ) can only be a set of independent solutions of the Schrödinger equation. Direct substitution of Eq. (2) for W' into Eq. (1) renders

$$\frac{a\phi + c\theta/2}{a\phi^2 + b\theta^2 + c\phi\theta}[-\hbar^2/(2m)\phi'' - (E - V)\phi]$$

$$+\frac{b\theta + c\phi/2}{a\phi^2 + b\theta^2 + c\phi\theta}[-\hbar^2/(2m)\theta'' - (E - V)\theta]$$

$$-\frac{[\mathcal{W}^2\hbar^2(ab - c^2/4)/(2m) - 1]}{(a\phi^2 + b\theta^2 + c\phi\theta)^2} = 0.\tag{3}$$

For the general solution for W', the real coefficients (a, b, c) are arbitrary within the limitations that $a, b > 0$ and from the Wronskian that $ab - c^2/4 > 0$. Hence, for generality the expressions within each of the three square brackets on the left side of Eq. (3) must vanish identically. The expressions within the first two of these square brackets manifest the Schrödinger equation, so the expressions within these two square brackets are identically zero if and only if ϕ and θ are solutions of the Schrödinger equation. The expression within third bracket vanishes identically if and only if the normalization of the Wronskian is such that $\mathcal{W}^2(\phi, \theta) = 2m/[\hbar^2(ab - c^2/4)]$. For $\mathcal{W}(\phi, \theta) \neq 0$, ϕ and θ must be independent solutions of the Schrödinger equation. Hence, ϕ and θ must form a set of independent solutions of the Schrödinger equation.

Let us investigate, first, the initial condition problem. The Schrödinger wave function is complex and is uniquely specified by initial conditions $\psi(x_o)$ and $\psi'(x_o)$. By the superposition principle, the Schrödinger wave function is described by $\psi = \alpha\phi + \beta\theta$ where α and β are coefficients uniquely specified, as well known, by the initial conditions as

$$\alpha = \frac{\psi(x_o)\theta'(x_o) - \psi'(x_o)\theta(x_o)}{\phi(x_o)\theta'(x_o) - \phi'(x_o)\theta(x_o)}$$

and

$$\beta = -\frac{\psi(x_o)\phi'(x_o) - \psi'(x_o)\phi(x_o)}{\phi(x_o)\theta'(x_o) - \phi'(x_o)\theta(x_o)}.$$

The coefficients α and β may be complex. The steady-state Schrödinger wave function can also be expressed by [12]

$$\begin{aligned}
\psi &= \frac{(2m)^{1/4}}{(W')^{1/2}[a - c^2/(4b)]^{1/2}} \exp(iW/\hbar) \\
&= \frac{(a\phi^2 + b\theta^2 + c\phi\theta)^{1/2}}{[a - c^2/(4b)]^{1/2}} \exp\left\{i\left[\arctan\left(\frac{b(\theta/\phi) + c/2}{(ab - c^2/4)^{1/2}}\right)\right]\right\} \\
&= [1 + ic/(4ab - c^2)^{1/2}]\phi + ib\theta/(ab - c^2/4)^{1/2}.
\end{aligned} \tag{4}$$

Thus, the relationships between the coefficients for steady-state Schrödinger wave functions and for the conjugate momentum are given by $\alpha = [1 + ic/(4ab - c^2)^{1/2}]$ and $\beta = ib/(ab - c^2/4)^{1/2}$. Specifying the initial conditions for the Schrödinger wave function along with the normalization of the Wronskian does indeed determine the coefficients (a, b, c) for the generalized Hamilton-Jacobi representation. Hence, the initial conditions for the wave function determine a unique trajectory for $W'(x)$ in phase space. Also, these initial conditions establish to within an integration constant, K, a unique W which is the generator of motion for a unique trajectory as a function of time, t, in configuration space as the equation of motion is the Hamilton-Jacobi transformation equation (often called Jacobi's theorem) $t - \tau = \partial W/\partial E$ where τ specifies the epoch.

We now consider the boundary value problem. The boundary value problem is not as simple. The solutions for boundary value problem, if they exist at all, need not be unique. As is well known for bound states, solutions for the Schrödinger wave function do exist for the energy eigenvalues. Not as well known, solutions for Hamilton's characteristic function for the trajectory representation of quantum mechanics exist if the action variable is quantized [4,11]. Specifically, we consider the bound state problem where $\psi \to 0$ as $x \to \pm\infty$. These are the bound state eigenfunctions which are unique. While the Schrödinger wave function is unique for bound states, the conjugate momentum is not [11]. In the generalized Hamilton-Jacobi representation of quantum mechanics, the boundary conditions for bound motion manifest a phase-space trajectory with turning points at $x = \pm\infty$ (exceptions to this include the infinitely deep square well where the turning points are at the edges of the well for the Schrödinger wave function does not penetrate the classically forbidden domain). This is accomplished by $W' \to 0$ as $x \to \pm\infty$. However, the generalized

Hamilton-Jacobi equation for the bound states is a nonlinear differential equation that has critical (singular) points at the very location where the boundary values are applied, i.e., $x = \pm\infty$. By Eq. (2), $W' \to 0$ as $x \to \pm\infty$ because at least one of the independent solutions, ϕ or θ, of the Schrödinger equation must be unbound as $x \to \pm\infty$. As the coefficients satisfy $a, b > 0$ and $ab > c^2/4$, the conjugate momentum exhibits a node as $x \to \pm\infty$ for all permitted values of a, b, and c [11]. Hence, the boundary values, $W'(x = \pm\infty) = 0$, for Eq. (1) permit non-unique phase-space trajectories for W' for energy eigenvalues or quantized action variables. Likewise, the trajectories in configuration space are not unique for the energy eigenvalue as the equation of motion, $t - \tau = \partial W/\partial E$, specifies a trajectory dependent upon the coefficients a, b and c.

We now show that these non-unique trajectories in phase space and configuration space manifest microstates of the Schrödinger wave function. For bound states in one dimension, the time-independent Schrödinger wave function may be real except for an inconsequential phase factor [14]. Bound states have the boundary values that $\psi(x = \pm\infty) = 0$. Let us choose ϕ to be the bound solution. Then $\psi = \alpha\phi$. The Schrödinger wave function can be represented in trigonometric form as [11]

$$
\begin{aligned}
\psi &= \frac{(2m)^{1/4}\cos(W/\hbar)}{(W')^{1/2}[a - c^2/(4b)]^{1/2}} \\
&= \frac{(a\phi^2 + b\theta^2 + c\phi\theta)^{1/2}}{[a - c^2/(4b)]^{1/2}} \cos\left[\arctan\left(\frac{b(\theta/\phi) + c/2}{(ab - c^2/4)^{1/2}}\right)\right] = \phi.
\end{aligned}
\tag{5}
$$

Thus, $\alpha = 1$ and $\beta = 0$ for all permitted values of the set (a, b, c). Each of these non-unique trajectories of energy E manifest a microstate of the Schrödinger wave function for the bound state. These microstates of energy E are specified by the set (a, b, c).

There is another explanation for our findings. For the unbound case, ψ is complex while W and W' are real. This is consistent with ψ being proportional to $(W')^{-1/2}\exp(iW/\hbar)$, cf. Eq. (4), even though a relationship exist between W and W'. But ψ may be represented as real in one dimension for bound states, cf. Eq. (5). Thus, there is some freedom in choosing W and W' which allows an uncountable number of different trajectories to be consistent with a particular bound-state eigenfunction.

We now understand in one dimension the reasons why for bound states the generalized Hamilton-Jacobi representation describes microstates not detected by the Schrödinger representation while for initial condition problems the two representations are equivalent. As the generalized Hamilton-Jacobi representation provides additional information identifying microstates, we must conclude that the Schrödinger wave function is not an exhaustive description of nonrelativistic quantum mechanics while the generalized Hamilton-Jacobi representation is so.

As the generalized Hamilton-Jacobi equation renders information regarding microstates while the Schrödinger equation does not, the two equations are not equivalent. The generalized Hamilton-Jacobi equation is the more fundamental.

3. HIGHER DIMENSIONS

Our results can be extended to higher dimensions if separation of variables is permitted. The existence of various bound-state trajectories for the same bound-state wave function in a separable coordinate system manifests a counter example showing that Schrödinger wave function is not the exhaustive description in higher dimensions. If the variables, including time, cannot be separated, the development of closed-form solutions is presently severely encumbered in either representations. Furthermore, closed form solutions for either representation are presently not known in general. Nevertheless, we may still discuss the more general problem. For stationary bound states, closed Dirichlet boundary conditions are sufficient to determine a unique, stable solution for the Schrödinger wave function. On the other hand, in the trajectory representation, the generalized Hamilton-Jacobi representation for the trajectory in three dimensions is given by the pair of equations [15]

$$\frac{\partial S}{\partial t} = -\frac{(\nabla S)^2}{2m} - V + \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R},$$

$$\frac{\partial R}{\partial t} = -\frac{1}{2m}(R\nabla^2 S + 2\nabla R \cdot \nabla S),$$

where S is Hamilton's principal function and R is the amplitude function in three dimensions corresponding to the Milne [4] or Pinney [5] amplitude function in one dimension. For systems independent of time, Lee has simplified the above pair of equations to [16]

$$\nabla^2 R + (2m/\hbar^2)(E - V)R - \lambda^2\kappa^2 R^{-3} = 0,$$

where λ is a normalization constant and κ is an expansion coefficient given by

$$\kappa = \exp\left(-\int^{\sigma} \nabla \cdot (\nabla W/|\nabla W|)\,d\sigma\right),$$

where $d\sigma$ is an element of arc length, $d\sigma^2 = dx^2 + dy^2 + dz^2$ in cartesian coordinates, along the gradient of W. (We note that in general the gradient of W is not necessarily co-axial with the trajectory [12].) The action variable for the generalized Hamilton-Jacobi representation in higher dimensions still has finite quantization. Therefore, the contribution of action along the trajectory in the classically forbidden region must be finite despite its infinite length out to the turning points at infinity. Accordingly, the conjugate momentum projected along the trajectory must decrease extremely rapidly to zero far in the classically forbidden region. Hence, the turning point has the characteristic of a node in the theory of nonlinear differential equations. This presents evidence that the trajectory representation for a bound state has a critical point in general at points where the Dirichlet boundary conditions are applied to the wave function which in turn indicates that an uncountable number of microstates (trajectories) for a bound states is possible.

POSTSCRIPT

A current investigation, not yet reported, examines the Goos-Hanchen effect in the trajectory representation of quantum mechanics for reflection off a semi-infinite rectangular barrier. The Schrödinger wave function, ψ, for sub-barrier energy, represents neither a bound particle, for such a particle is not confined to a finite region [17], nor an unbound particle, for ψ is monotonically dampened in a semi-infinite domain. For trajectories with sub- barrier energy, such a barrier generates a nodal singularity in the trajectory and concurrently a zero in ψ at a point infinitely deep in the barrier. This single nodal singularity is sufficient, by itself, to induce microstates of the Schrödinger wave function. Thus, we conclude that if any nodal singularity exists in the trajectory representation, then microstates exist and ψ is not an exhaustive description of nonrelativistic quantum phenomenon.

REFERENCES

1. A. Zwaan, thesis, *Intensitäten im Ca-Funkenspektrum*, Utrecht, 1929.
2. E. C. Kemble, *The Fundamental Principles of Quantum Mechanics with Elementary Applications* (Dover, New York, 1937), p. 95.
3. A. Mesiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. I, p. 232.
4. W. E. Milne, *Phys. Rev.* **35**, 863 (1930).
5. E. Pinney, *Proc. Am. Math. Soc.* **1**, 681 (1950).
6. C. J. Eliezer and A. Gray, *SIAM J. Appl. Math.* **30**, 463 (1976).
7. H. J. Korsch and H. Laurent, *J. Phys.* **B 14**, 4213 (1981).

8. J. Killingbeck, *J. Phys.* **A 13**, L231 (1980).

9. H. R. Lewis, Jr., *Phys. Rev. Lett.* **18**, 510 (1967).

10. E. R. Floyd, *Phys. Rev.* **D 25**, 1547 (1982).

11. E. R. Floyd, *Phys. Rev.* **D 34**, 3246 (1986).

12. E. R. Floyd, *Phys. Essays* **7**, 135 (1994).

13. E. R. Floyd, *Ann. Fond. Louis de Broglie* **20**, 263 (1995).

14. L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Addison-Wesley, Reading, Massachusetts, 1958) pp. 52 and 160.

15. D. Bohm, *Phys. Rev.* **85**, 166 (1952).

16. R. A. Lee, *J. Phys.* **A 15**, 2761 (1982); *Opt. Acta* **31**, 1119 (1984).

17. *McGraw-Hill Dictionary of Physics and Mathematics*, D. N. Lapedes, ed. (McGraw-Hill, New York, 1978), p. 108.